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AI-Driven Materials Genome: Accelerated Discovery of Multi-Functional Sensing Materials

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Abstract

Multi-functional sensing materials play a critical role in advanced technologies, including medical devices, environmental monitoring, and smart infrastructure. The discovery and development of these materials using traditional methods is often time-consuming and costly, relying predominantly on experimental testing.

The materials genome approach, which integrates computational data, simulations, and predictive analyses, provides a pathway to accelerate the materials discovery process. In this article, a roadmap for the design of multi-functional sensing materials is presented, encompassing data-driven strategies, predictive algorithms, and experimental feedback loops.

Limitations such as data scarcity, model uncertainty, and challenges in result interpretability are also discussed, along with perspectives on developing faster and more efficient methods for materials discovery and optimization. **Keywords:** materials genome, sensor, materials design, ai-driven, dataset.

The purpose of the research

The primary goal is to address the inefficiencies in traditional sensing material discovery which is often costly and time-consuming. This study aims to: Integrate computational modeling and AI to identify optimal material compositions.

•Bridge the gap between atomic-scale structures and device-level functional responses.

•Establish a robust roadmap for designing high-performance, multifunctional sensors through data-driven mapping.

By implementing this AI-driven framework, we achieve:

Accelerated Workflow: Transformed sensing material discovery from time-consuming "trial-and-error" to a rapid, predictable computational process.

Enhanced Mapping: Established a reliable link between micro-structural features and macro-scale sensing performance for multifunctional materials.

Superior Design: Enabled the identification of high-performance materials.

Research method

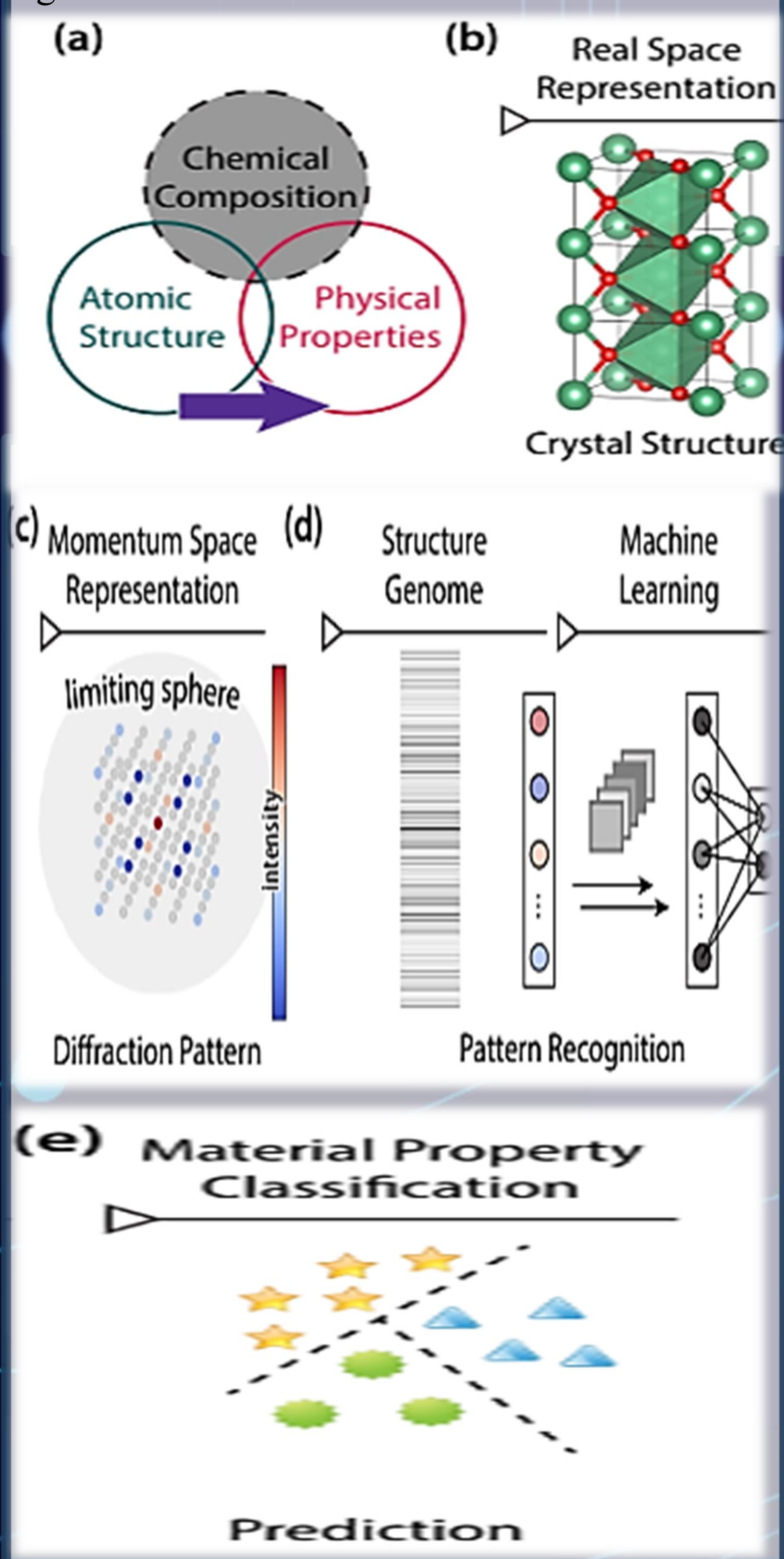
The framework follows a four-pillar cycle:

1.Material Databases: Leveraging standardized datasets (e.g., Materials Project, AFLOW) to train predictive models.

2.High-Throughput Computation: Using Density Functional Theory (DFT) to generate reliable data for unexplored compounds.

3.AI & ML Integration: Employing Graph Neural Networks (GNNs) and Bayesian Optimization to capture complex non-linear relationships between structure and properties.

4.Experimental Validation: A closed-loop feedback system where AI-driven predictions are synthesized and tested to refine model accuracy. Figure 1 illustrates this process in general.



conclusion

The integration of the Materials Genome framework with artificial intelligence and machine learning provides an innovative approach for the discovery and design of multi-functional sensing materials. By combining experimental and simulation data, analyzing complex structure–property–function (SPF) relationships, and simultaneously predicting multiple properties, this approach enables the rapid and targeted identification of material compositions with optimal performance.

While challenges such as limited standardized data, data heterogeneity, and uncertainty management remain, this methodology offers a new pathway to reduce traditional trial-and-error processes and to design multi-functional sensors with high sensitivity, stability, and predictable performance.

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